Chapter 8

Single-particle propagator in many-particle systems

In analogy to the case of the sp problem it is possible to consider a corresponding propagator in the many-body system. The definition of this quantity for fermions is given in Sec. 8.1. This definition involves the use of the Heisenberg picture in quantum mechanics [Sakurai (1994); Messiah (1999)]. For completeness some of the relevant results related to various pictures in Quantum Mechanics are collected in App. A. The propagator is defined in terms of either adding or removing a particle from the correlated ground state. The removal process is a new feature not present in the sp problem. Complementary information is contained in these removal and addition amplitudes. Both are accessible experimentally, the addition process in the form of elastic scattering from the correlated ground state and the removal process in the form of coincidence experiments of the form $(e,2e)$ from atoms and $(e,e'p)$ from nuclei. Various incarnations of the sp propagator in the many-body system are discussed. A particularly relevant one is given by the Lehmann representation in Sec. 8.2 and requires a Fourier transform to the energy formulation. An interesting contact with experimental data can me be made for the imaginary part of the sp propagator. The relevant quantities are the spectral functions describing the removal and addition probability density of particles with specified quantum numbers to and from the correlated ground state. These quantities are introduced in Sec. 8.3. In Sec. 8.4 it is shown that expectation values of one-body operators in the ground state can be obtained from the one-body density matrix which is related to the "hole" part of the sp propagator. In addition to all one-body expectation values, it is possible to obtain the energy of the ground state from the hole part of the sp propagator in the case that the Hamiltonian contains at most two-body operators. Simple examples for the sp propgator in a noninteracting system are discussed in

Sec. 8.5. A simple discussion of knockout reactions and their relation to spectral functions is presented in Sec. 8.6. Experimental data from the $(e, 2e)$ reaction on atoms are discussed in Sec. 8.7. Corresponding data for the $(e, e'p)$ reaction on nuclei are reviewed in Sec. 8.8. From the comparision with experiment a clear "sp" picture of the atom and the nucleus arises that further motivates the development of the propagator description of the many-fermion system.

8.1 Fermion single-particle propagator

The sp propagator in a many-particle system is defined as an expectation value with respect to the exact ground state of the system of A particles, of an operator which represents both particle propagation as well as hole propagation. The latter term is naturally absent in the one-particle problem.

$$G(\alpha,\beta;t,t') = -\frac{i}{\hbar}\frac{\langle\Psi_0^A|\,\mathcal{T}[a_{\alpha_H}(t)a^\dagger_{\beta_H}(t')]\,|\Psi_0^A\rangle}{\langle\Psi_0^A|\Psi_0^A\rangle}, \tag{8.1}$$

where $|\Psi_0^A\rangle$ is the Heisenberg ground state for the A-particle system and E_0^A the corresponding eigenvalue

$$\hat{H}\,|\Psi_0^A\rangle = E_0^A\,|\Psi_0^A\rangle. \tag{8.2}$$

The particle addition and removal operators in the definition of the sp propagator are given in the Heisenberg picture by

$$a_{\alpha_H}(t) = e^{\frac{i}{\hbar}\hat{H}t}a_\alpha e^{-\frac{i}{\hbar}\hat{H}t} \tag{8.3}$$

and

$$a^\dagger_{\alpha_H}(t) = e^{\frac{i}{\hbar}\hat{H}t}a^\dagger_\alpha e^{-\frac{i}{\hbar}\hat{H}t}, \tag{8.4}$$

respectively. The time-ordering operation $\mathcal{T}$ is defined here to include a sign change when two fermion operators are interchanged and can be written using step functions as

$$\mathcal{T}[a_{\alpha_H}(t)a^\dagger_{\beta_H}(t')] = \theta(t-t')a_{\alpha_H}(t)a^\dagger_{\beta_H}(t') - \theta(t'-t)a^\dagger_{\beta_H}(t')a_{\alpha_H}(t). \tag{8.5}$$

This operation therefore puts operators with the later time to the left of earlier operators and includes a sign when a change of order is required. For now we will assume that the correlated ground state is normalized although the form of normalization used in Eq. (8.1) will be used in Ch. 9

when the perturbation expansion of the sp propagator is developed. Using the definition of the Heisenberg picture operators and the time-ordering operation for fermion operators one obtains

$$\begin{aligned} G(\alpha,\beta;t-t') = -\frac{i}{\hbar}\Big\{ &\theta(t-t') e^{\frac{i}{\hbar}E_0^A(t-t')} \left\langle \Psi_0^A \right| a_\alpha e^{-\frac{i}{\hbar}\hat{H}(t-t')} a_\beta^\dagger \left| \Psi_0^A \right\rangle \\ &-\theta(t'-t) e^{\frac{i}{\hbar}E_0^A(t'-t)} \left\langle \Psi_0^A \right| a_\beta^\dagger e^{-\frac{i}{\hbar}\hat{H}(t'-t)} a_\alpha \left| \Psi_0^A \right\rangle \Big\} \end{aligned} \tag{8.6}$$

$$\begin{aligned} = -\frac{i}{\hbar}\Big\{ &\theta(t-t') \sum_m e^{\frac{i}{\hbar}(E_0^A - E_m^{A+1})(t-t')} \left\langle \Psi_0^A \right| a_\alpha \left| \Psi_m^{A+1} \right\rangle \left\langle \Psi_m^{A+1} \right| a_\beta^\dagger \left| \Psi_0^A \right\rangle \\ &-\theta(t'-t) \sum_n e^{\frac{i}{\hbar}(E_0^A - E_n^{A-1})(t'-t)} \left\langle \Psi_0^A \right| a_\beta^\dagger \left| \Psi_n^{A-1} \right\rangle \left\langle \Psi_n^{A-1} \right| a_\alpha \left| \Psi_0^A \right\rangle \Big\}. \end{aligned}$$

As expected, the propagator depends only on the time difference $t-t'$. Note that the completeness of the exact eigenstates of $\hat{H}$ for both the $A+1$ as well as the $A-1$ system has been used together with

$$\hat{H} \left| \Psi_m^{A+1} \right\rangle = E_m^{A+1} \left| \Psi_m^{A+1} \right\rangle \tag{8.7}$$

and

$$\hat{H} \left| \Psi_n^{A-1} \right\rangle = E_n^{A-1} \left| \Psi_n^{A-1} \right\rangle . \tag{8.8}$$

While the similarity with Eq. (7.6) is evident, it is also clear that Eq. (8.6) contains relevant information about the many-body system.

8.2 Lehmann representation

As in the sp problem, one can introduce the FT of the sp propagator which is more convenient for practical calculations but also brings out the information that is contained in the sp propagator more clearly

$$G(\alpha,\beta;E) = \int_{-\infty}^{\infty} d(t-t')\ e^{\frac{i}{\hbar}E(t-t')}\ G(\alpha,\beta;t-t'). \tag{8.9}$$

As before, it is recommended to use the integral representation of the step-function as given in Eq. (7.7). The result of this FT can be expressed in various equivalent ways. The FT of the last expression for $G(\alpha,\beta;t-t')$

in Eq. (8.6) yields

$$\begin{aligned} G(\alpha,\beta;E) &= \sum_m \frac{\left\langle \Psi_0^A \right| a_\alpha \left| \Psi_m^{A+1} \right\rangle \left\langle \Psi_m^{A+1} \right| a_\beta^\dagger \left| \Psi_0^A \right\rangle}{E - (E_m^{A+1} - E_0^A) + i\eta} \\ &+ \sum_n \frac{\left\langle \Psi_0^A \right| a_\beta^\dagger \left| \Psi_n^{A-1} \right\rangle \left\langle \Psi_n^{A-1} \right| a_\alpha \left| \Psi_0^A \right\rangle}{E - (E_0^A - E_n^{A-1}) - i\eta} \\ &= \left\langle \Psi_0^A \right| a_\alpha \frac{1}{E - (\hat{H} - E_0^A) + i\eta} a_\beta^\dagger \left| \Psi_0^A \right\rangle \\ &+ \left\langle \Psi_0^A \right| a_\beta^\dagger \frac{1}{E - (E_0^A - \hat{H}) - i\eta} a_\alpha \left| \Psi_0^A \right\rangle . \end{aligned} \tag{8.10}$$

The first equality is known as the Lehmann representation [Lehmann (1954)] of the sp propagator. The last line is obtained by removing the complete set of exact $A+1$-eigenstates in the first term and the complete set of $A-1$-eigenstates in the second one, after replacing the eigenvalues E_m^{A+1} and E_n^{A-1} by $\hat{H}$. Note that **any** sp basis can be used in this formulation of the propagator. Many texts choose to specialize either to coordinate space or momentum representation. This does not always represent the appropriate choice especially when dealing with finite systems where comparisons with experimental results are readily possible. It is also instructive to compare this form of the sp propagator with the corresponding one for the sp problem (see Eq. (7.9)). Apart from the hole term which is naturally absent in the sp case there is a clear similarity between the two results. Indeed, the matrix elements involving the addition and removal operators obey Schrödinger-like equations as will be discussed in more detail later.

8.3 Spectral functions

In the case of finite systems, one can relate essentially all the information contained in the sp propagator to relevant experimental results. Consider first the information in the denominator of the first equality in Eq. (8.10). The positions of the poles signal the location of the excited states in the $A+1$ or $A-1$ particle systems with respect to the ground state of the A particle system. Note that it should be possible to reach those states by the addition (or removal) of a particle with sp quantum numbers α to (or from) the ground state of this system. In this context it is useful to visualize the addition or removal of a particle as a physical process that can be realized experimentally. Second, the information in the numerator determines the distribution of the corresponding transition strength from the ground state of the A particle system to these states in the $A \pm 1$ systems. This information is a crucial measure of the strength of the correlations in the system as they induce behavior which deviates from the independent particle model. A good tool to develop intuition for the effect of correlations on sp properties is provided by the spectral function. The hole part of the spectral function at energy E is the combined probability density for removing a particle with quantum numbers α from the ground state while leaving the remaining $A-1$-system at an energy $E_n^{A-1} = E_0^A - E$. This quantity is proportional to the imaginary part of the diagonal element of the sp propagator

$$\begin{aligned} S_h(\alpha, E) &= \frac{1}{\pi} \text{ Im } G(\alpha, \alpha; E) & E \leq \epsilon_F^- \\ &= \sum_n \left| \left\langle \Psi_n^{A-1} \right| a_\alpha \left| \Psi_0^A \right\rangle \right|^2 \delta(E - (E_0^A - E_n^{A-1})). & (8.11) \end{aligned}$$

A detailed presentation of experimental information about this quantity in atoms and nuclei will be discussed in Secs. 8.7 and 8.8, respectively. A similar probability density exists for the addition of a particle with quantum numbers α leaving the $A+1$-system at energy $E_m^{A+1} = E_0^A + E$ is obtained from

$$\begin{aligned} S_p(\alpha, E) &= -\frac{1}{\pi} \text{ Im } G(\alpha, \alpha; E) & E \geq \epsilon_F^+ \\ &= \sum_m \left| \left\langle \Psi_m^{A+1} \right| a_\alpha^\dagger \left| \Psi_0^A \right\rangle \right|^2 \delta(E - (E_m^{A+1} - E_0^A)). & (8.12) \end{aligned}$$

This quantity is referred to as the particle spectral function. The corresponding Fermi energies introduced in Eqs. (8.11) and (8.12) are given by

$$\epsilon_F^- = E_0^A - E_0^{A-1} \quad (8.13)$$

$$\epsilon_F^+ = E_0^{A+1} - E_0^A. \quad (8.14)$$

In obtaining the imaginary part of the propagator the very useful identity

$$\frac{1}{E \pm i\eta} \;=\; \mathcal{P}\frac{1}{E} \;\mp\; i\pi\delta(E) \quad (8.15)$$

has been used, where the symbol $\mathcal{P}$ denotes the principal value. The above expressions for the spectral functions are particularly useful for analyzing finite systems where discrete bound states exist and for certain problems involving band structure, localization or external magnetic fields in condensed matter systems. In finite systems, like nuclei, there can be a considerable difference between ϵ_F^- and ϵ_F^+. In infinite systems which are not superfluids or superconductors this difference vanishes in the thermodynamic limit.

The occupation number of a sp state α can be obtained from the hole part of the spectral function by evaluating

$$\begin{aligned} n(\alpha) &= \left\langle \Psi_0^A \right| a_\alpha^\dagger a_\alpha \left| \Psi_0^A \right\rangle = \sum_n \left| \left\langle \Psi_n^{A-1} \right| a_\alpha \left| \Psi_0^A \right\rangle \right|^2 \\ &= \int_{-\infty}^{\epsilon_F^-} dE \ \sum_n \left| \left\langle \Psi_n^{A-1} \right| a_\alpha \left| \Psi_0^A \right\rangle \right|^2 \delta(E - (E_0^A - E_n^{A-1})) \\ &= \int_{-\infty}^{\epsilon_F^-} dE \ S_h(\alpha, E). \end{aligned} \tag{8.16}$$

In a similar way one can obtain the depletion number from the particle part of the spectral function

$$\begin{aligned} d(\alpha) &= \left\langle \Psi_0^A \right| a_\alpha a_\alpha^\dagger \left| \Psi_0^A \right\rangle = \sum_m \left| \left\langle \Psi_m^{A+1} \right| a_\alpha^\dagger \left| \Psi_0^A \right\rangle \right|^2 \\ &= \int_{\epsilon_F^+}^{\infty} dE \ \sum_m \left| \left\langle \Psi_m^{A+1} \right| a_\alpha^\dagger \left| \Psi_0^A \right\rangle \right|^2 \delta(E - (E_m^{A+1} - E_0^A)) \\ &= \int_{\epsilon_F^+}^{\infty} dE \ S_p(\alpha, E). \end{aligned} \tag{8.17}$$

An important sum rule exists for $n(\alpha)$ and $d(\alpha)$ which can be obtained by using the anticommutation relation for a_α and $a_\alpha^\dagger$

$$n(\alpha) + d(\alpha) = \left\langle \Psi_0^A \right| a_\alpha^\dagger a_\alpha \left| \Psi_0^A \right\rangle + \left\langle \Psi_0^A \right| a_\alpha a_\alpha^\dagger \left| \Psi_0^A \right\rangle = \langle \Psi_0^A | \Psi_0^A \rangle = 1. \tag{8.18}$$

This distribution between occupation and emptiness of a sp orbital in the correlated ground state is a sensitive measure of the strength of correlations provided a suitable sp basis is chosen to be discussed in Secs. 8.7 and 8.8.

8.4 Expectation values of operators in the correlated ground state

The sp propagator will also provide the expectation value of any one-body operator in the ground state

$$\left\langle \Psi_0^A \right| \hat{O} \left| \Psi_0^A \right\rangle = \sum_{\alpha,\beta} \langle\alpha| O |\beta\rangle \left\langle \Psi_0^A \right| a_\alpha^\dagger a_\beta \left| \Psi_0^A \right\rangle = \sum_{\alpha,\beta} \langle\alpha| O |\beta\rangle \, n_{\alpha\beta}. \quad (8.19)$$

Here, $n_{\alpha\beta}$ is the one-body density matrix element which can be be obtained from the sp propagator using the Lehmann representation

$$\begin{aligned} n_{\beta\alpha} &= \int \frac{dE}{2\pi i} \; e^{iE\eta} \; G(\alpha,\beta;E) \qquad (8.20) \\ &= \int \frac{dE}{2\pi i} \; e^{iE\eta} \; \sum_n \frac{\left\langle \Psi_0^A \right| a_\beta^\dagger \left| \Psi_n^{A-1} \right\rangle \left\langle \Psi_n^{A-1} \right| a_\alpha \left| \Psi_0^A \right\rangle}{E - (E_0^A - E_n^{A-1}) - i\eta} \\ &= \sum_n \left\langle \Psi_0^A \right| a_\beta^\dagger \left| \Psi_n^{A-1} \right\rangle \left\langle \Psi_n^{A-1} \right| a_\alpha \left| \Psi_0^A \right\rangle = \left\langle \Psi_0^A \right| a_\beta^\dagger a_\alpha \left| \Psi_0^A \right\rangle . \end{aligned}$$

Note the convergence factor in the integral with infinitesimal η which requires closing the contour in the upper half of the complex E-plane. Therefore, only the (nondiagonal) hole part of the spectral amplitude contributes. An equivalent result is obtained by directly using the imaginary part of the propagator

$$n_{\beta\alpha} = \frac{1}{\pi} \int_{-\infty}^{\epsilon_F^-} dE \;\; \mathrm{Im}\; G(\alpha,\beta;E) = \left\langle \Psi_0^A \right| a_\beta^\dagger a_\alpha \left| \Psi_0^A \right\rangle . \qquad (8.21)$$

With this result for $n_{\beta\alpha}$ it is clear that Eq. (8.19) yields any expectation value of a one-body operator in the correlated ground state.

Surprisingly, the energy of the ground state can also be obtained from the sp propagator provided that, as has been assumed up to now, there are only two-body interactions between the particles. This is a quite remarkable result first clarified by [Galitskii and Migdal (1958)] and later applied to finite systems by [Koltun (1972); Koltun (1974)]. Again, only the hole part of the propagator is required for this result. Consider the following integral

$$\begin{aligned} I_\alpha &= \frac{1}{\pi} \int_{-\infty}^{\epsilon_F^-} dE \; E \;\; \mathrm{Im}\; G(\alpha,\alpha;E) = \int_{-\infty}^{\epsilon_F^-} dE \; E \; S_h(\alpha,E) \qquad (8.22) \\ &= \sum_m (E_0^A - E_m^{A-1}) \left\langle \Psi_0^A \right| a_\alpha^\dagger \left| \Psi_m^{A-1} \right\rangle \left\langle \Psi_m^{A-1} \right| a_\alpha \left| \Psi_0^A \right\rangle \end{aligned}$$

$$= \left\langle \Psi_0^A \right| a_\alpha^\dagger a_\alpha \hat{H} \left| \Psi_0^A \right\rangle - \sum_m \left\langle \Psi_0^A \right| a_\alpha^\dagger E_m^{A-1} \left| \Psi_m^{A-1} \right\rangle \left\langle \Psi_m^{A-1} \right| a_\alpha \left| \Psi_0^A \right\rangle$$
$$= \left\langle \Psi_0^A \right| a_\alpha^\dagger a_\alpha \hat{H} \left| \Psi_0^A \right\rangle - \left\langle \Psi_0^A \right| a_\alpha^\dagger \hat{H} a_\alpha \left| \Psi_0^A \right\rangle = \left\langle \Psi_0^A \right| a_\alpha^\dagger [a_\alpha, \hat{H}] \left| \Psi_0^A \right\rangle$$

The commutator in Eq. (8.22) can again be evaluated using Eqs. (2.34) and (2.42) with the result

$$[a_\alpha, \hat{H}] = \sum_\beta \langle \alpha | T | \beta \rangle \, a_\beta + \sum_{\beta\gamma\delta} (\alpha\beta|V|\gamma\delta) a_\beta^\dagger a_\delta a_\gamma. \tag{8.23}$$

Inserting Eq. (8.23) into (8.22) finally yields

$$I_\alpha = \sum_\beta \langle \alpha | T | \beta \rangle \left\langle \Psi_0^A \right| a_\alpha^\dagger a_\beta \left| \Psi_0^A \right\rangle + \sum_{\beta\gamma\delta} (\alpha\beta|V|\gamma\delta) \; \left\langle \Psi_0^A \right| a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \left| \Psi_0^A \right\rangle . \tag{8.24}$$

Summing this expression over α one then obtains

$$\sum_\alpha I_\alpha = \left\langle \Psi_0^A \right| \hat{T} \left| \Psi_0^A \right\rangle + 2 \left\langle \Psi_0^A \right| \hat{V} \left| \Psi_0^A \right\rangle . \tag{8.25}$$

Combining the result of Eq. (8.25) with the expectation value for the kinetic energy using Eq. (8.19) one obtains the desired result

$$\begin{aligned} E_0^A &= \left\langle \Psi_0^A \right| \hat{H} \left| \Psi_0^A \right\rangle \\ &= \frac{1}{2\pi} \int_{-\infty}^{\epsilon_F^-} dE \; \sum_{\alpha,\beta} \{ \langle \alpha | T | \beta \rangle + \; E \; \delta_{\alpha,\beta} \} \; \mathrm{Im} \; G(\beta, \alpha; E) \\ &= \frac{1}{2} \sum_{\alpha,\beta} \langle \alpha | T | \beta \rangle \, n_{\alpha\beta} + \frac{1}{2} \sum_\alpha \int_{-\infty}^{\epsilon_F^-} dE \; E \; S_h(\alpha, E), \end{aligned} \tag{8.26}$$

where the validity of the last equality can be checked by inserting the definition of $S_h(\alpha, E)$ given in Eq. (8.11).

8.5 Propagator for noninteracting systems

In the case the many-particle problem does not contain a two-body interaction operator, for example with Hamiltonian $\hat{H}_0$ and ground state $\left|\Phi_0^A\right\rangle$, the sp propagator becomes

$$G^{(0)}(\alpha, \beta; t - t') = -\frac{i}{\hbar} \left\langle \Phi_0^A \right| \mathcal{T}[a_{\alpha_I}(t) a_{\beta_I}^\dagger(t')] \left| \Phi_0^A \right\rangle , \tag{8.27}$$

where $\left|\Phi_0^A\right\rangle$ is the nondegenerate ground state of $\hat{H}_0$ for A particles with eigenvalue

$$E^A_{\Phi_0} = \sum_{\alpha<F} \varepsilon_\alpha \tag{8.28}$$

as in Eq. (3.9) and therefore

$$\hat{H}_0 \left|\Phi_0^A\right\rangle = E^A_{\Phi_0} \left|\Phi_0^A\right\rangle . \tag{8.29}$$

The extension to treating propagators for open shell systems is non-trivial and not well developed. It will not be further discussed here. For the present considerations the state $\left|\Phi_0^A\right\rangle$ can correspond to the Slater determinant of an infinite Fermi system, a closed-shell atom, or a closed-shell nucleus. The particle addition and removal operators in the definition of the so-called unperturbed sp propagator, are given then given by the equivalent of Eqs. (8.3) and (8.4) with the replacement $\hat{H} \to \hat{H}_0$. This substitution yields these operators in the so-called interaction picture (see App. A) given by

$$a_{\alpha_I}(t) = e^{\frac{i}{\hbar}\hat{H}_0 t} a_\alpha e^{-\frac{i}{\hbar}\hat{H}_0 t} \tag{8.30}$$

and

$$a^\dagger_{\alpha_I}(t) = e^{\frac{i}{\hbar}\hat{H}_0 t} a^\dagger_\alpha e^{-\frac{i}{\hbar}\hat{H}_0 t}, \tag{8.31}$$

respectively. Assuming that H_0 is diagonal in the sp basis $\{|\alpha\rangle\}$ and using the corresponding interaction picture operators given by Eqs. (A.15) and (A.16) together with the time-ordering operation for fermion operators, one obtains

$$\begin{aligned} G^{(0)}(\alpha,\beta;t-t') = -\frac{i}{\hbar}\big\{&\theta(t-t')\delta_{\alpha,\beta}\theta(\alpha-F)e^{-\frac{i}{\hbar}\varepsilon_\alpha(t-t')} \\ &- \theta(t'-t)\delta_{\alpha,\beta}\theta(F-\alpha)e^{\frac{i}{\hbar}\varepsilon_\alpha(t'-t)}\big\} \end{aligned} \tag{8.32}$$

which represents the propagation of a particle or a hole on top of the non-interacting ground state. One should note as in Ch. 3 that the states with one particle added or removed with quantum numbers associated with H_0 are correspondingly eigenstates of $\hat{H}_0$ according to

$$\hat{H}_0 a^\dagger_\alpha \left|\Phi_0^A\right\rangle = (E^A_{\Phi_0} + \varepsilon_\alpha) a^\dagger_\alpha \left|\Phi_0^A\right\rangle \qquad \alpha > F \tag{8.33}$$

and

$$\hat{H}_0 a_\alpha \left|\Phi_0^A\right\rangle = (E^A_{\Phi_0} - \varepsilon_\alpha) a_\alpha \left|\Phi_0^A\right\rangle \qquad \alpha < F, \tag{8.34}$$

respectively. Choosing another sp basis leads to a slightly more involved result which can be related to the present one by a double basis transformation both for the particle addition as well as the particle removal operator according to Eqs. (2.58) and (2.59).

Again it is fruitful to consider the FT of the unperturbed sp propagator

$$G^{(0)}(\alpha,\beta;E) = \delta_{\alpha,\beta}\left\{ \frac{\theta(\alpha - F)}{E - \varepsilon_\alpha + i\eta} + \frac{\theta(F - \alpha)}{E - \varepsilon_\alpha - i\eta} \right\}. \tag{8.35}$$

This result is again equivalent to the result for the exact propagator given in Eq. (8.11) with $\hat{H}$ replaced by $\hat{H}_0$ and $\left|\Psi_0^A\right\rangle$ by $\left|\Phi_0^A\right\rangle$

$$\begin{aligned} G^{(0)}(\alpha,\beta;E) &= \left\langle \Phi_0^A \right| a_\alpha \frac{1}{E - (\hat{H}_0 - E^A_{\Phi_0}) + i\eta} a^\dagger_\beta \left|\Phi_0^A\right\rangle \\ &\quad + \left\langle \Phi_0^A \right| a^\dagger_\beta \frac{1}{E - (E^A_{\Phi_0} - \hat{H}_0) - i\eta} a_\alpha \left|\Phi_0^A\right\rangle . \end{aligned} \tag{8.36}$$

The spectral functions for the non-interacting system are particularly simple. Using again the sp basis $\{|\alpha\rangle\}$ which diagonalizes H_0, one has the following hole spectral function

$$\begin{aligned} S_h(\alpha,E) &= \frac{1}{\pi}\mathrm{Im}\ G^{(0)}(\alpha,\alpha;E) \\ &= \delta(E - \varepsilon_\alpha)\ \theta(F - \alpha) \qquad\qquad E < \varepsilon_F^{(0)^-} \end{aligned} \tag{8.37}$$

and particle spectral function

$$\begin{aligned} S_p(\alpha,E) &= -\frac{1}{\pi}\mathrm{Im}\ G^{(0)}(\alpha,\alpha;E) \\ &= \delta(E - \varepsilon_\alpha)\ \theta(\alpha - F) \qquad\qquad E > \varepsilon_F^{(0)^+}. \end{aligned} \tag{8.38}$$

This shows that the strength in the unperturbed spectral function occurs at the sp energies which correspond to the eigenvalues of the sp Hamiltonian H_0. The sp states that are occupied yield contributions to the hole spectral function, those that are empty contribute to the particle spectral function. In this independent particle model description for an atom, a nucleus, or a Fermi gas, the hole spectral function displays δ-function peaks with strength 1 which corresponds to the certainty that it is possible to remove a particle from such an occupied orbital. The same holds for the particle spectral function where this certainty relates to the possibility of adding a particle to an empty orbit. The simplicity of these results is related to the choice of the sp basis. In another sp basis the numerators change while the position of the poles in the sp propagator does not change. As an example, consider the sp propagator in the $\{|\boldsymbol{r}m_s\rangle\}$ representation

$$G^{(0)}(\boldsymbol{r}m_s, \boldsymbol{r}'m_s'; E) = \langle \Phi_0 | \, a_{\boldsymbol{r}m_s} \frac{1}{E - (\hat{H}_0 - E^A_{\Phi_0}) + i\eta} a^\dagger_{\boldsymbol{r}'m_s'} \, |\Phi_0\rangle$$
$$+ \langle \Phi_0 | \, a^\dagger_{\boldsymbol{r}'m_s'} \frac{1}{E - (E^A_{\Phi_0} - \hat{H}_0) - i\eta} a_{\boldsymbol{r}m_s} \, |\Phi_0\rangle \tag{8.39}$$
$$= \sum_\alpha \left\{ \frac{\langle \boldsymbol{r}m_s|\alpha\rangle\langle\alpha|\boldsymbol{r}'m_s'\rangle\theta(\alpha - F)}{E - \varepsilon_\alpha + i\eta} + \frac{\langle \boldsymbol{r}m_s|\alpha\rangle\langle\alpha|\boldsymbol{r}'m_s'\rangle\theta(F - \alpha)}{E - \varepsilon_\alpha - i\eta} \right\}.$$

Note that the numerators in Eq. (8.39) contain again the relevant sp wave functions which in this simple example represent the transition matrix elements of the particle addition and removal operators in the coordinate representation. Occupation numbers are most easily evaluated in the $\{|\alpha\rangle\}$ basis. The resulting occupation numbers then read (not surprisingly)

$$n(\alpha) = \int_{-\infty}^{\varepsilon_F^{(0)-}} dE \; \delta(E - \varepsilon_\alpha) \; \theta(F - \alpha) = \theta(F - \alpha). \tag{8.40}$$

8.6 Direct knock-out reactions

The hole spectral function introduced in Sec. 8.3 can be experimentally observed in so-called knock-out reactions. The general idea is to transfer a large amount of momentum and energy to a particle of a bound A-particle system (e.g. an electron in an atom or molecule, or a nucleon in a nucleus). The particle is then ejected from the system, and one ends up with a fast-moving particle and a bound $(A-1)$-particle system. By observing the momentum of the ejected particle it is then possible the reconstruct the spectral function of the system, provided that the interaction between the ejected particle and the remainder is sufficiently weak.

Let's assume that the A-particle system is initially in its ground state,

$$|\Psi_i\rangle = \left|\Psi_0^A\right\rangle, \tag{8.41}$$

and makes a transition to a final A-particle eigenstate

$$|\Psi_f\rangle = a^\dagger_{\boldsymbol{p}} \left|\Psi_n^{A-1}\right\rangle, \tag{8.42}$$

composed of a bound $(A-1)$-particle eigenstate, $\left|\Psi_n^{A-1}\right\rangle$, and a particle with momentum $\boldsymbol{p}$.

For simplicity we consider the transition matrix elements for a scalar external probe $\rho(\boldsymbol{q}) = \sum_{j=1}^{A} \exp\left(i\boldsymbol{q}\cdot\boldsymbol{r}_j/\hbar\right)$, which transfers momentum $\boldsymbol{q}$ to a particle. Suppressing other possible sp quantum numbers, like *e.g.* spin, the second-quantized form of this operator is given by

$$\hat{\rho}(\boldsymbol{q}) = \sum_{\boldsymbol{p},\boldsymbol{p}'} \langle \boldsymbol{p}| \exp\left(i\boldsymbol{q}\cdot\boldsymbol{r}/\hbar\,|\boldsymbol{p}'\rangle\, a^\dagger_{\boldsymbol{p}} a_{\boldsymbol{p}'} = \sum_{\boldsymbol{p}} a^\dagger_{\boldsymbol{p}} a_{\boldsymbol{p}-\boldsymbol{q}}. \tag{8.43}$$

The transition matrix element now becomes

$$\begin{aligned}
\langle \Psi_f |\, \hat{\rho}(\boldsymbol{q})\, | \Psi_i \rangle &= \sum_{\boldsymbol{p}'} \left\langle \Psi_n^{A-1} \right| a_{\boldsymbol{p}} a^\dagger_{\boldsymbol{p}'} a_{\boldsymbol{p}'-\boldsymbol{q}} \left| \Psi_0^A \right\rangle \\
&= \sum_{\boldsymbol{p}'} \left\langle \Psi_n^{A-1} \right| \delta_{\boldsymbol{p}',\boldsymbol{p}} a_{\boldsymbol{p}'-\boldsymbol{q}} + a^\dagger_{\boldsymbol{p}'} a_{\boldsymbol{p}'-\boldsymbol{q}} a_{\boldsymbol{p}} \left| \Psi_0^A \right\rangle \\
&\approx \left\langle \Psi_n^{A-1} \right| a_{\boldsymbol{p}-\boldsymbol{q}} \left| \Psi_0^A \right\rangle .
\end{aligned} \tag{8.44}$$

The last line is obtained in the so-called *Impulse Approximation*, where it is assumed that the ejected particle is the one that has absorbed the momentum from the external field. This is a very good approximation whenever the momentum $\boldsymbol{p}$ of the ejectile is much larger than typical momenta for the particles in the bound states; the neglected term in Eq. (8.44) is then very small, as it involves the removal of a particle with momentum $\boldsymbol{p}$ from $|\ \Psi_0^A\rangle$.

There is one other assumption in the derivation: the fact that the final eigenstate of the A-particle system was written in the form of Eq. (8.42), i.e. a plane-wave state for the ejectile on top of an $(A-1)$-particle eigenstate. This is again a good approximation if the ejectile momentum is large enough, as can be understood by rewriting the Hamiltonian in the A-particle system as

$$H_A = \sum_{i=1}^{A} \frac{\boldsymbol{p}_i^2}{2m} + \sum_{i<j=1}^{A} V(i,j) = H_{A-1} + \frac{\boldsymbol{p}_A^2}{2m} + \sum_{i=1}^{A-1} V(i,A). \tag{8.45}$$

The last term in Eq. (8.45) represents the *Final State Interaction*, or the interaction between the ejected particle A and the other particles $1\ldots A-1$. If the relative momentum between particle A and the others is large enough their mutual interaction can be neglected, and $H_A \approx H_{A-1} + \boldsymbol{p}_A^2/2m$.

The result (8.44) is called the *Plane Wave Impulse Approximation* or PWIA knock-out amplitude, for obvious reasons, and is precisely a removal amplitude (in the momentum representation) appearing in the Lehmann representation of the sp propagator (see Eq. (8.10)).

The cross section of the knock-out reaction, where the momentum and energy of the ejected particle and the probe are either measured or known, ia according to Fermi's golden rule proportional to

$$d\sigma \sim \sum_n \delta(\hbar\omega + E_i - E_f) |\langle \Psi_f | \hat{\rho}(\boldsymbol{q}) | \Psi_i \rangle|^2, \tag{8.46}$$

where the energy-conserving δ-function contains the energy transfer $\hbar\omega$ of the probe, and the initial and final energies of the system are $E_i = E_0^A$ and $E_f = E_n^{A-1} + \boldsymbol{p}^2/2m$, respectively. Note that the internal state of the residual $A-1$ system is not measured, hence the summation over n in Eq. (8.46).

Defining the missing momentum $\boldsymbol{p}_m$ and missing energy E_m of the knock-out reaction as[1]

$$\boldsymbol{p}_{miss} = \boldsymbol{p} - \boldsymbol{q} \tag{8.47}$$

and

$$E_{miss} = \boldsymbol{p}^2/2m - \hbar\omega = E_0^A - E_n^{A-1}, \tag{8.48}$$

respectively, the PWIA knock-out cross section can be rewritten as

$$\begin{aligned} d\sigma &\sim \sum_n \delta(E_{miss} - E_0^A + E_n^{A-1}) |\langle \Psi_n^{A-1} | a_{\boldsymbol{p}_{miss}} | \Psi_0^A \rangle|^2 \\ &= S_h(\boldsymbol{p}_{miss}, E_{miss}). \end{aligned} \tag{8.49}$$

The PWIA cross section is therefore exactly proportional to the hole spectral function defined in Eq. (8.11). This is of course only true in the PWIA, but when the deviations of the impulse approximation and the effects of the final state interaction are small as for atoms or well under control as for nuclei, it is possible to obtain precise experimental information on the hole spectral function of the system under study.

In many cases the A-particle target system is probed by its interaction with an external electromagnetic radiation field. This is obviously the case when the target is placed in a real photon beam, but it is also true when a beam of electrons is incident on the target, e.g. in nuclear $(e, e'p)$ reactions, or $(e, 2e)$ reactions on atoms, molecules and solids. In that case the scattering process of the electron off a particle in the target can be described on a deeper level as the exchange of a virtual photon between the electron and a target particle. In general, a photon is characterized by its 4-momentum

[1] We will neglect here the recoil of the residual $A-1$ system, i.e. we assume the mass of the A and $A-1$ system to be much heavier than the mass m of the ejected particle.

$(\omega, \boldsymbol{q})$ (using $\hbar = c = 1$) and its polarization 4-vector $(\epsilon_0, \boldsymbol{\epsilon})$. A real photon has $\omega = q$, $\epsilon_0 = 0$ and a tranverse polarization 3-vector, $\boldsymbol{\epsilon} \cdot \boldsymbol{q} = 0$. A virtual photon has $\omega < q$ and a polarization 4-vector that has a longitudinal component, $\boldsymbol{\epsilon} \cdot \boldsymbol{q} \neq 0$.

The corresponding interaction hamiltonian reads

$$\hat{H}_{\text{int}}(t) = \int d\boldsymbol{r} \exp\left[i(\boldsymbol{q} \cdot \boldsymbol{r} - \omega t)\right] \left(\epsilon_0 \hat{\rho}(\boldsymbol{r}) - \boldsymbol{\epsilon} \cdot \hat{\boldsymbol{J}}(\boldsymbol{r})\right), \tag{8.50}$$

$$= \exp\left[i\omega t\right] \left(\epsilon_0 \hat{\rho}(\boldsymbol{q}) - \boldsymbol{\epsilon} \cdot \hat{\boldsymbol{J}}(\boldsymbol{q})\right), \tag{8.51}$$

where $\hat{\rho}$ and $\hat{\boldsymbol{J}}$ are the charge density operator and current density operator of the A-particle system. The charge density corresponds to the scalar probe that was above. The vector nature of the current density somewhat complicates the discussion, but it can be shown that also in this case the important proportionality in Eq. (8.49) holds [Frullani and Mougey (1984)].

8.7 Comparison with $(e, 2e)$ data for atoms

8.8 Comparison with $(e, e'p)$ data for nuclei

8.9 Exercises